Author Index to Volume 170

Abbé, J.Ch., see J.C. Machado 170 (1993) 257
Aguilar, M.A., see F.J. Olivares del Valle 170 (1993) 161
Allouche, A.R., G. Wannous and M. Aubert-Frécon, A ligand-field approach for the low-lying states of Ca, Sr and Ba monohalides 170 (1993) 11
Aubert-Frécon, M., see A.R. Allouche 170 (1993) 11

Beidoun, A., see A. Penzkofer 170 (1993) 139
Benderskii, V.A., D.E. Makarov and P.G. Grinevich, Quantum chemical dynamics in two dimensions 170 (1993) 275
Billing, G.D., see R.E. Kolesnick 170 (1993) 201
Borgis, D. and J.T. Hynes, Dynamical theory of proton tunneling transfer rates in solution: general formulation 170 (1993) 315
Boukheddaden, K., J. Linares, A. Bousseksou, J. Nasser, H. Rabah and F. Varret, Intramolecular aspects of the electron transfer in the biferrocenium mixed-valence cation, using PKS theory 170 (1993) 47
Bousseksou, A., see K. Boukheddaden 170 (1993) 47
Bree, A. and R. Zwarich, Matrix-induced two-photon absorption in anthracene 170 (1993) 185
Brion, C.E., see W.F. Chan 170 (1993) 81
Brion, C.E., see W.F. Chan 170 (1993) 99
Brion, C.E., see W.F. Chan 170 (1993) 111
Brion, C.E., see W.F. Chan 170 (1993) 123
Brochon, J.C., see P. Lianos 170 (1993) 235
Brown, R. and C. Von Borczyskowski, The behaviour of trapping after diffusion by tunneling in disordered systems 170 (1993) 57
Buenker, R.J., see L. Chantranupong 170 (1993) 167

Cai, Z.-L., Ab initio study of the X $^1\Sigma^+$ and A $^1\Pi$ states of the cyanate anion (NCO^-) 170 (1993) 33
Carvalho, C.F., see J.C. Machado 170 (1993) 257
Češpiva, L., see J. Vojtík 170 (1993) 37
Chan, W.F., G. Cooper, R.N.S. Sodhi and C.E. Brion, Absolute optical oscillator strengths for discrete and continuum photoabsorption of molecular nitrogen (11–200 eV) 170 (1993) 81
Chan, W.F., G. Cooper and C.E. Brion, Absolute optical oscillator strengths for the photoabsorption of molecular oxygen (5–30 eV) at high resolution 170 (1993) 99
Chan, W.F., G. Cooper and C.E. Brion, Absolute optical oscillator strengths for the photoabsorption of nitric oxide (5–30 eV) at high resolution 170 (1993) 111
Chan, W.F., G. Cooper and C.E. Brion, Absolute optical oscillator strengths for discrete and continuum photoabsorption of carbon monoxide (7–200 eV) and transition moments for the X $^1\Sigma^+ \rightarrow$ A $^1\Pi$ system 170 (1993) 123
Chantranupong, L., G. Hirsch, R.J. Buenker and M.A. Dillon, Configuration interaction calculations of the vertical electronic spectrum of silane 170 (1993) 167
Contador, J.C., see F.J. Olivares del Valle 170 (1993) 161

Author Index to Volume 170

Abbé, J.Ch., see J.C. Machado 170 (1993) 257
Aguilar, M.A., see F.J. Olivares del Valle 170 (1993) 161
Allouche, A.R., G. Wannous and M. Aubert-Frécon, A ligand-field approach for the low-lying states of Ca, Sr and Ba monohalides 170 (1993) 11
Aubert-Frécon, M., see A.R. Allouche 170 (1993) 11

Beidoun, A., see A. Penzkofer 170 (1993) 139
Benderskii, V.A., D.E. Makarov and P.G. Grinevich, Quantum chemical dynamics in two dimensions 170 (1993) 275
Billing, G.D., see R.E. Kolesnick 170 (1993) 201
Borgis, D. and J.T. Hynes, Dynamical theory of proton tunneling transfer rates in solution: general formulation 170 (1993) 315
Boukheddaden, K., J. Linares, A. Bousseksou, J. Nasser, H. Rabah and F. Varret, Intramolecular aspects of the electron transfer in the biferrocenium mixed-valence cation, using PKS theory 170 (1993) 47
Bousseksou, A., see K. Boukheddaden 170 (1993) 47
Bree, A. and R. Zwarich, Matrix-induced two-photon absorption in anthracene 170 (1993) 185
Brion, C.E., see W.F. Chan 170 (1993) 81
Brion, C.E., see W.F. Chan 170 (1993) 99
Brion, C.E., see W.F. Chan 170 (1993) 111
Brion, C.E., see W.F. Chan 170 (1993) 123
Brochon, J.C., see P. Lianos 170 (1993) 235
Brown, R. and C. Von Borczyskowski, The behaviour of trapping after diffusion by tunneling in disordered systems 170 (1993) 57
Buenker, R.J., see L. Chantranupong 170 (1993) 167

Cai, Z.-L., Ab initio study of the X $^1\Sigma^+$ and A $^1\Pi$ states of the cyanate anion (NCO^-) 170 (1993) 33
Carvalho, C.F., see J.C. Machado 170 (1993) 257
Češpiva, L., see J. Vojtík 170 (1993) 37
Chan, W.F., G. Cooper, R.N.S. Sodhi and C.E. Brion, Absolute optical oscillator strengths for discrete and continuum photoabsorption of molecular nitrogen (11–200 eV) 170 (1993) 81
Chan, W.F., G. Cooper and C.E. Brion, Absolute optical oscillator strengths for the photoabsorption of molecular oxygen (5–30 eV) at high resolution 170 (1993) 99
Chan, W.F., G. Cooper and C.E. Brion, Absolute optical oscillator strengths for the photoabsorption of nitric oxide (5–30 eV) at high resolution 170 (1993) 111
Chan, W.F., G. Cooper and C.E. Brion, Absolute optical oscillator strengths for discrete and continuum photoabsorption of carbon monoxide (7–200 eV) and transition moments for the X $^1\Sigma^+ \rightarrow$ A $^1\Pi$ system 170 (1993) 123
Chantranupong, L., G. Hirsch, R.J. Buenker and M.A. Dillon, Configuration interaction calculations of the vertical electronic spectrum of silane 170 (1993) 167
Contador, J.C., see F.J. Olivares del Valle 170 (1993) 161

Cooper, G., see W.F. Chan 170 (1993) 81
Cooper, G., see W.F. Chan 170 (1993) 99
Cooper, G., see W.F. Chan 170 (1993) 111
Cooper, G., see W.F. Chan 170 (1993) 123

Daré, A.-M., see A. Filali-Mouhim 170 (1993) 23
Dillon, M.A., see L. Chantranupong 170 (1993) 167
Duplâtre, G., see J.C. Machado 170 (1993) 257

Filali-Mouhim, A., A.-M. Daré, J.-M. Lopez-Castillo and J.-P. Jay-Gerin, Electron delocalization and transfer induced by a time-dependent potential: exact treatment of a simple model – transfer 170 (1993) 23

García Cuesta, I., A. Sánchez de Merás and I. Nebot Gil, Binding and isomerization energies for the Cu/CN and Cu(I)CN interactions 170 (1993) 1
Goldanskii, V.I., see C.A. Wight 170 (1993) 393
Gordon, E.B., V.V. Khmelenko, A.A. Pelmenev, E.A. Popov, O.F. Pugachev and A.F. Shestakov, Metastable impurity-helium solid phase. Experimental and theoretical evidence 170 (1993) 411
Grellmann, K.H., see U. Kensy 170 (1993) 381
Grinevich, P.G., see V.A. Benderskii 170 (1993) 275
Grossmann, F. and P. Hänggi, ac-Driven quantum decay 170 (1993) 295

Hänggi, P., see F. Grossmann 170 (1993) 295
Herbich, J. and A. Kapturkiewicz, Radiative electron transfer in aryl derivatives of dimethylanilines 170 (1993) 221
Hermansson, K., Coordination effects on the stretching vibration of the OH^- ion 170 (1993) 177
Hirade, T. and O.E. Mogensen, Dependence of the yield of the short-lived ortho-Ps state on the concentration of CCl_4 in hexane 170 (1993) 249
Hirsch, G., see L. Chantranupong 170 (1993) 167
Hrdina, R., see S. Luňák Jr. 170 (1993) 77
Hynes, J.T., see D. Borgis 170 (1993) 315

Ito, Y., see M. Kusakabe 170 (1993) 243
Ivanov, G.K. and M.A. Kozhushner, Asymptotics of many-electron wavefunctions and calculation of tunnel transitions 170 (1993) 303

Jay-Gerin, J.-P., see A. Filali-Mouhim 170 (1993) 23
Jonker, S.A., see J.M. Warman 170 (1993) 359

Kapturkiewicz, A., see J. Herbich 170 (1993) 221
Kensy, U., M. Mosquera González and K.H. Grellmann, Tunnel effects on inter- and intramolecular hydrogen transfer reactions of transient dihydro- and hexahydrocarbazoles 170 (1993) 381
Khmelenko, V.V., see E.B. Gordon 170 (1993) 411
Klinger, M.I. and S.N. Taraskin, Thermally activated configurational tunneling at trapping and recombination in glassy semiconductors 170 (1993) 437
Kolesnick, R.E. and G.D. Billing, Rate constants for vibrational transitions in hydrogen and isotopes 170 (1993) 201

Kozhushner, M.A., see G.K. Ivanov 170 (1993) 303
Kroon, J., see J.M. Warman 170 (1993) 359
Kurfürst, A., see S. Luňák Jr. 170 (1993) 67
Kurfürst, A., see S. Luňák Jr. 170 (1993) 77
Kusakabe, M., Y. Ito and I. Tokue, Formation of CCl ($A^2\Delta$) by electron impact on $CXCl_3$ (X=H, F, Cl, Br) 170 (1993) 243
Kuthan, J., see S. Luňák Jr. 170 (1993) 67
Kuthan, J., see S. Luňák Jr. 170 (1993) 77

Lianos, P., J.C. Brochon and P. Tauc, Behavior of the rate constant for reactions in restricted spaces: case of luminescence quenching in water-in-oil microemulsions 170 (1993) 235
Linares, J., see K. Boukheddaden 170 (1993) 47
Lopez-Castillo, J.-M., see A. Filali-Mouhim 170 (1993) 23
Luňák Jr., S., M. Nepraš, A. Kurfürst and J. Kuthan, Photophysics of PBD derivatives. I. The fluorescence of para-biphenylyl-substituted 2-(biphenyl-4′-yl)-5-phenyl-1,3,4-oxadiazoles 170 (1993) 67
Luňák Jr., S., M. Nepraš, R. Hrdina, A. Kurfürst and J. Kuthan, Photophysics of PBD derivatives. II. The character of the lowest excited triplet state of 2-(biphenyl-4′-yl)-5-phenyl-1,3,4-oxadiazole 170 (1993) 77

Machado, J.C., C.F. Carvalho, W.F. Magalhães, A. Marques Netto, J.Ch. Abbé and G. Duplâtre, Positronium formation and inhibition in binary solid solutions on Al(III) and Co(III) tris(acetylacetonates) 170 (1993) 257
Magalhães, W.F., see J.C. Machado 170 (1993) 257
Makarov, D.E., see V.A. Benderskii 170 (1993) 275
Marques Netto, A., see J.C. Machado 170 (1993) 257
Misochko, E.Y., see C.A. Wight 170 (1993) 393
Mogensen, O.E., see T. Hirade 170 (1993) 249
Mosquera González, M., see U. Kensy 170 (1993) 381

Nasser, J., see K. Boukheddaden 170 (1993) 47
Nebot Gil, I., see I. García Cuesta 170 (1993) 1
Nepraš, M., see S. Luňák Jr. 170 (1993) 67
Nepraš, M., see S. Luňák Jr. 170 (1993) 77

Oevering, H., see J.M. Warman 170 (1993) 359
Olivares del Valle, F.J., M.A. Aguilar and J.C. Contador, Cavity boundaries in the ab initio polarizable continuum model 170 (1993) 161
Oliver, A.M., see J.M. Warman 170 (1993) 359

Paddon-Row, M.N., see J.M. Warman 170 (1993) 359
Paidarová, I., see J. Vojtík 170 (1993) 37
Pelmenev, A.A., see E.B. Gordon 170 (1993) 411
Penzkofer, A., A. Beidoun and S. Speiser, Singlet excited-state absorption of eosin Y 170 (1993) 139
Persson, B.J., see L.G.M. Pettersson 170 (1993) 149
Pettersson, L.G.M. and B.J. Persson, Effects of core correlation on atomic and dimeric phosphorus 170 (1993) 149

Pollak, E. and D. Proselkov, Quantum variational transition state theory revisited 170 (1993) 265
Popov, E.A., see E.B. Gordon 170 (1993) 411
Proselkov, D., see E. Pollak 170 (1993) 265
Pugachev, O.F., see E.B. Gordon 170 (1993) 411

Rabah, H., see K. Boukheddaden 170 (1993) 47

Samios, J. and H. Stassen, Time correlation functions of liquid OCS. A molecular dynamics simulation study 170 (1993) 193
Sánchez de Merás, A., see I. García Cuesta 170 (1993) 1
Šavrda, J., see J. Vojtík 170 (1993) 37
Shestakov, A.F., see E.B. Gordon 170 (1993) 411
Siebrand, W., see Z.K. Smedarchina 170 (1993) 347
Smedarchina, Z.K. and W. Siebrand, Multimode approach to hydrogen tunneling 170 (1993) 347
Smit, K.J., see J.M. Warman 170 (1993) 359
Sodhi, R.N.S., see W.F. Chan 170 (1993) 81
Speiser, S., see A. Penzkofer 170 (1993) 139
Stassen, H., see J. Samios 170 (1993) 193
Syutkin, V.M., see V.A. Tolkatchev 170 (1993) 427

Taraskin, S.N., see M.I. Klinger 170 (1993) 437
Tauc, P., see P. Lianos 170 (1993) 235
Tokue, I., see M. Kusakabe 170 (1993) 243
Tolkatchev, V.A., V.M. Syutkin and V.L. Vyazovkin, The role of local motions in the kinetic peculiarities of atomic tunneling in solids 170 (1993) 427

Varret, F., see K. Boukheddaden 170 (1993) 47
Verhoeven, J.W., see J.M. Warman 170 (1993) 359
Vetoshkin, E.V., see C.A. Wight 170 (1993) 393
Vojtík, J., I. Paidarová, L. Češpiva and J. Šavrda, Energy derivative method in MRD CI calculation of rovibrational dependence of nuclear quadrupole coupling constants of diatomic molecules. Application to $^{7}Li^{2}H$ in the $X\ ^{1}\Sigma^{+}$ and $A\ ^{1}\Sigma^{+}$ states 170 (1993) 37
Vojtík, J., Calculations of static characteristics of the ionization event in low-energy $He(2^{3}S)$–H_2 collisions 170 (1993) 209
Von Borczyskowski, C., see R. Brown 170 (1993) 57
Vyazovkin, V.L., see V.A. Tolkatchev 170 (1993) 427

Wannous, G., see A.R. Allouche 170 (1993) 11
Warman, J.M., K.J. Smit, S.A. Jonker, J.W. Verhoeven, H. Oevering, J. Kroon, M.N. Paddon-Row and A.M. Oliver, Intramolecular charge separation and recombination in non-polar environments via long-distance electron transfer through saturated hydrocarbon barriers 170 (1993) 359
Wight, C.A., E.Y. Misochko, E.V. Vetoshkin and V.I. Goldanskii, Tunneling dynamics and spatial correlations of long chain growth in solid-state photochlorination of ethylene at low temperatures 170 (1993) 393

Zwarich, R., see A. Bree 170 (1993) 185

Subject Index to Volume 170

Methods

Theoretical

Classical mechanics
Quantum chemical dynamics in two dimensions, V.A. Benderskii, D.E. Makarov and P.G. Grinevich 170 (1993) 275

Coupling schemes and perturbative treatments
Binding and isomerization energies for the Cu/CN and Cu(I)CN interactions, I. García Cuesta, A. Sánchez de Merás and I. Nebot Gil 170 (1993) 1
A ligand-field approach for the low-lying states of Ca, Sr and Ba monohalides, A.R. Allouche, G. Wannous and M. Aubert-Frécon 170 (1993) 11
ac-Driven quantum decay, F. Grossmann and P. Hänggi 170 (1993) 295
Thermally activated configurational tunneling at trapping and recombination in glassy semiconductors, M.I. Klinger and S.N. Taraskin 170 (1993) 437

Transport quantum mechanics
Electron delocalization and transfer induced by a time-dependent potential: exact treatment of a simple model – transfer, A. Filali-Mouhim, A.-M. Daré, J.-M. Lopez-Castillo and J.-P. Jay-Gerin 170 (1993) 23
ac-Driven quantum decay, F. Grossmann and P. Hänggi 170 (1993) 295
Asymptotics of many-electron wavefunctions and calculation of tunnel transitions, G.K. Ivanov and M.A. Kozhushner 170 (1993) 303
Dynamical theory of proton tunneling transfer rates in solution: general formulation, D. Borgis and J.T. Hynes 170 (1993) 315

Equilibrium statistical mechanics
Quantum variational transition state theory revisited, E. Pollak and D. Proselkov 170 (1993) 265

Ab initio schemes for stationary properties
Binding and isomerization energies for the Cu/CN and Cu(I)CN interactions, I. García Cuesta, A. Sánchez de Merás and I. Nebot Gil 170 (1993) 1
Ab initio study of the X $^1\Sigma^+$ and A $^1\Pi$ states of the cyanate anion (NCO^-), Z.-L. Cai 170 (1993) 33
Energy derivative method in MRD CI calculation of rovibrational dependence of nuclear quadrupole coupling constants of diatomic molecules. Application to $^7Li^2H$ in the X $^1\Sigma^+$ and A $^1\Sigma^+$ states, J. Vojtík, I. Paidarová, L. Češpiva and J. Šavrda 170 (1993) 37
Effects of core correlation on atomic and dimeric phosphorus, L.G.M. Pettersson and B.J. Persson 170 (1993) 149

Cavity boundaries in the ab initio polarizable continuum model, F.J. Olivares del Valle, M.A. Aguilar and J.C. Contador 170 (1993) 161
Configuration interaction calculations of the vertical electronic spectrum of silane, L. Chantranupong, G. Hirsch, R.J. Buenker and M.A. Dillon 170 (1993) 167
Coordination effects on the stretching vibration of the OH^- ion, K. Hermansson 170 (1993) 177

Computational and simulation methods
Electron delocalization and transfer induced by a time-dependent potential: exact treatment of a simple model – transfer, A. Filali-Mouhim, A.-M. Daré, J.-M. Lopez-Castillo and J.-P. Jay-Gerin 170 (1993) 23
Intramolecular aspects of the electron transfer in the biferrocenium mixed-valence cation, using PKS theory, K. Boukheddaden, J. Linares, A. Bousseksou, J. Nasser, H. Rabah and F. Varret 170 (1993) 47
The behaviour of trapping after diffusion by tunneling in disordered systems, R. Brown and C. Von Borczyskowski 170 (1993) 57
Effects of core correlation on atomic and dimeric phosphorus, L.G.M. Pettersson and B.J. Persson 170 (1993) 149
Cavity boundaries in the ab initio polarizable continuum model, F.J. Olivares del Valle, M.A. Aguilar and J.C. Contador 170 (1993) 161
Matrix-induced two-photon absorption in anthracene, A. Bree and R. Zwarich 170 (1993) 185
Time correlation functions of liquid OCS. A molecular dynamics simulation study, J. Samios and H. Stassen 170 (1993) 193
Tunneling dynamics and spatial correlations of long chain growth in solid-state photochlorination of ethylene at low temperatures, C.A. Wight, E.Y. Misochko, E.V. Vetoshkin and V.I. Goldanskii 170 (1993) 393
Metastable impurity-helium solid phase. Experimental and theoretical evidence, E.B. Gordon, V.V. Khmelenko, A.A. Pelmenev, E.A. Popov, O.F. Pugachev and A.F. Shestakov 170 (1993) 411

Molecular dynamics and scattering theory
Rate constants for vibrational transitions in hydrogen and isotopes, R.E. Kolesnick and G.D. Billing 170 (1993) 201
Calculations of static characteristics of the ionization event in low-energy $He(2^3S)$–H_2 collisions, J. Vojtík 170 (1993) 209
Quantum variational transition state theory revisited, E. Pollak and D. Proselkov 170 (1993) 265
Asymptotics of many-electron wavefunctions and calculation of tunnel transitions, G.K. Ivanov and M.A. Kozhushner 170 (1993) 303
Dynamical theory of proton tunneling transfer rates in solution: general formulation, D. Borgis and J.T. Hynes 170 (1993) 315
Multimode approach to hydrogen tunneling, Z.K. Smedarchina and W. Siebrand 170 (1993) 347

Experimental

Magnetic resonances
The role of local motions in the kinetic peculiarities of atomic tunneling in solids, V.A. Tolkatchev, V.M. Syutkin and V.L. Vyazovkin 170 (1993) 427

Microwave spectroscopy
ac-Driven quantum decay, F. Grossmann and P. Hänggi 170 (1993) 295

Infrared spectroscopy
Tunneling dynamics and spatial correlations of long chain growth in solid-state photochlorination of ethylene at low temperatures, C.A. Wight, E.Y. Misochko, E.V. Vetoshkin and V.I. Goldanskii 170 (1993) 393

Visible and UV spectroscopy
Photophysics of PBD derivatives. I. The fluorescence of para-biphenylyl-substituted 2-(biphenyl-4′-yl)-5-phenyl-1,3,4-oxadiazoles, S. Luňák Jr., M. Nepraš, A. Kurfürst and J. Kuthan 170 (1993) 67
Photophysics of PBD derivatives. II. The character of the lowest excited triplet state of 2-(biphenyl-4′-yl)-5-phenyl-1,3,4-oxadiazole, S. Luňák Jr., M. Nepraš, R. Hrdina, A. Kurfürst and J. Kuthan 170 (1993) 77
Absolute optical oscillator strengths for discrete and continuum photoabsorption of molecular nitrogen (11–200 eV), W.F. Chan, G. Cooper, R.N.S. Sodhi and C.E. Brion 170 (1993) 81
Absolute optical oscillator strengths for the photoabsorption of molecular oxygen (5–30 eV) at high resolution, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 99
Absolute optical oscillator strengths for the photoabsorption of nitric oxide (5–30 eV) at high resolution, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 111
Absolute optical oscillator strengths for discrete and continuum photoabsorption of carbon monoxide (7–200 eV) and transition moments for the $X\,^1\Sigma^+ \rightarrow A\,^1\Pi$ system, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 123

Fluorescence spectroscopy
Photophysics of PBD derivatives. I. The fluorescence of para-biphenylyl-substituted 2-(biphenyl-4′-yl)-5-phenyl-1,3,4-oxadiazoles, S. Luňák Jr., M. Nepraš, A. Kurfürst and J. Kuthan 170 (1993) 67
Radiative electron transfer in aryl derivatives of dimethylanilines, J. Herbich and A. Kapturkiewicz 170 (1993) 221
Behavior of the rate constant for reactions in restricted spaces: case of luminescence quenching in water-in-oil microemulsions, P. Lianos, J.C. Brochon and P. Tauc 170 (1993) 235

Electron impact spectroscopy
Formation of CCl ($A^2\Delta$) by electron impact on $CXCl_3$ (X=H, F, Cl, Br), M. Kusakabe, Y. Ito and I. Tokue 170 (1993) 243

Laser methods
Radiative electron transfer in aryl derivatives of dimethylanilines, J. Herbich and A. Kapturkiewicz 170 (1993) 221
Intramolecular charge separation and recombination in non-polar environments via long-distance electron transfer through saturated hydrocarbon barriers, J.M. Warman, K.J. Smit, S.A. Jonker, J.W. Verhoeven, H. Oevering, J. Kroon, M.N. Paddon-Row and A.M. Oliver 170 (1993) 359

Picosecond spectroscopy
Singlet excited-state absorption of eosin Y, A. Penzkofer, A. Beidoun and S. Speiser 170 (1993) 139

Non-linear optical spectroscopy
Singlet excited-state absorption of eosin Y, A. Penzkofer, A. Beidoun and S. Speiser 170 (1993) 139
Matrix-induced two-photon absorption in anthracene, A. Bree and R. Zwarich 170 (1993) 185

Atomic and molecular beam techniques
Metastable impurity-helium solid phase. Experimental and theoretical evidence, E.B. Gordon, V.V. Khmelenko, A.A. Pelmenev, E.A. Popov, O.F. Pugachev and A.F. Shestakov 170 (1993) 411

Time-resolved experiments
Singlet excited-state absorption of eosin Y, A. Penzkofer, A. Beidoun and S. Speiser 170 (1993) 139
Dependence of the yield of the short-lived ortho-Ps state on the concentration of CCl_4 in hexane, T. Hirade and O.E. Mogensen 170 (1993) 249
Intramolecular charge separation and recombination in non-polar environments via long-distance electron transfer through saturated hydrocarbon barriers, J.M. Warman, K.J. Smit, S.A. Jonker, J.W. Verhoeven, H. Oevering, J. Kroon, M.N. Paddon-Row and A.M. Oliver 170 (1993) 359
Tunnel effects on inter- and intramolecular hydrogen transfer reactions of transient dihydro- and hexahydrocarbazoles, U. Kensy, M. Mosquera González and K.H. Grellmann 170 (1993) 381

Radiolysis
Positronium formation and inhibition in binary solid solutions on Al(III) and Co(III) tris(acetylacetonates), J.C. Machado, C.F. Carvalho, W.F. Magalhães, A. Marques Netto, J.Ch. Abbé and G. Duplâtre 170 (1993) 257

Mössbauer spectroscopy
Intramolecular aspects of the electron transfer in the biferrocenium mixed-valence cation, using PKS theory, K. Boukheddaden, J. Linares, A. Bousseksou, J. Nasser, H. Rabah and F. Varret 170 (1993) 47

Measurement of macroscopic variables
Positronium formation and inhibition in binary solid solutions on Al(III) and Co(III) tris(acetylacetonates), J.C. Machado, C.F. Carvalho, W.F. Magalhães, A. Marques Netto, J.Ch. Abbé and G. Duplâtre 170 (1993) 257

Objects

Bulk systems

Gases
Ab initio study of the X $^1\Sigma^+$ and A $^1\Pi$ states of the cyanate anion (NCO^-), Z.-L. Cai 170 (1993) 33
Rate constants for vibrational transitions in hydrogen and isotopes, R.E. Kolesnick and G.D. Billing 170 (1993) 201

Liquids neat
Time correlation functions of liquid OCS. A molecular dynamics simulation study, J. Samios and H. Stassen 170 (1993) 193

Liquids mixtures and solutions
Behavior of the rate constant for reactions in restricted spaces: case of luminescence quenching in water-in-oil microemulsions, P. Lianos, J.C. Brochon and P. Tauc 170 (1993) 235
Dependence of the yield of the short-lived ortho-Ps state on the concentration of CCl_4 in hexane, T. Hirade and O.E. Mogensen 170 (1993) 249

Crystals

–mixed
The behaviour of trapping after diffusion by tunneling in disordered systems, R. Brown and C. Von Borczyskowski 170 (1993) 57
Matrix-induced two-photon absorption in anthracene, A. Bree and R. Zwarich 170 (1993) 185
Positronium formation and inhibition in binary solid solutions on Al(III) and Co(III) tris(acetylacetonates), J.C. Machado, C.F. Carvalho, W.F. Magalhães, A. Marques Netto, J.Ch. Abbé and G. Duplâtre 170 (1993) 257
Tunneling dynamics and spatial correlations of long chain growth in solid-state photochlorination of ethylene at low temperatures, C.A. Wight, E.Y. Misochko, E.V. Vetoshkin and V.I. Goldanskii 170 (1993) 393

Glasses
The role of local motions in the kinetic peculiarities of atomic tunneling in solids, V.A. Tolkatchev, V.M. Syutkin and V.L. Vyazovkin 170 (1993) 427

Semiconductors
Thermally activated configurational tunneling at trapping and recombination in glassy semiconductors, M.I. Klinger and S.N. Taraskin 170 (1993) 437

Surfaces
Asymptotics of many-electron wavefunctions and calculation of tunnel transitions, G.K. Ivanov and M.A. Kozhushner 170 (1993) 303

Microscopic systems

Atoms
Effects of core correlation on atomic and dimeric phosphorus, L.G.M. Pettersson and B.J. Persson 170 (1993) 149

Molecules (neutral and ionic)
Ab initio study of the X $^1\Sigma^+$ and A $^1\Pi$ states of the cyanate anion (NCO^-), Z.-L. Cai 170 (1993) 33
Energy derivative method in MRD CI calculation of rovibrational dependence of nuclear quadrupole coupling constants of diatomic molecules. Application to $^7Li^2H$ in the X $^1\Sigma^+$ and A $^1\Sigma^+$ states, J. Vojtík, I. Paidarová, L. Češpiva and J. Šavrda 170 (1993) 37
Intramolecular aspects of the electron transfer in the biferrocenium mixed-valence cation, using PKS theory, K. Boukheddaden, J. Linares, A. Bousseksou, J. Nasser, H. Rabah and F. Varret 170 (1993) 47
Effects of core correlation on atomic and dimeric phosphorus, L.G.M. Pettersson and B.J. Persson 170 (1993) 149

Calculations of static characteristics of the ionization event in low-energy He(2^3S)–H_2 collisions, J. Vojtík 170 (1993) 209
Dynamical theory of proton tunneling transfer rates in solution: general formulation, D. Borgis and J.T. Hynes 170 (1993) 315
Multimode approach to hydrogen tunneling, Z.K. Smedarchina and W. Siebrand 170 (1993) 347

–diatomic
A ligand-field approach for the low-lying states of Ca, Sr and Ba monohalides, A.R. Allouche, G. Wannous and M. Aubert-Frécon 170 (1993) 11
Energy derivative method in MRD CI calculation of rovibrational dependence of nuclear quadrupole coupling constants of diatomic molecules. Application to $^7Li^2H$ in the X $^1\Sigma^+$ and A $^1\Sigma^+$ states, J. Vojtík, I. Paidarová, L. Češpiva and J. Šavrda 170 (1993) 37
Absolute optical oscillator strengths for discrete and continuum photoabsorption of molecular nitrogen (11–200 eV), W.F. Chan, G. Cooper, R.N.S. Sodhi and C.E. Brion 170 (1993) 81
Absolute optical oscillator strengths for the photoabsorption of molecular oxygen (5–30 eV) at high resolution, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 99
Absolute optical oscillator strengths for the photoabsorption of nitric oxide (5–30 eV) at high resolution, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 111
Absolute optical oscillator strengths for discrete and continuum photoabsorption of carbon monoxide (7–200 eV) and transition moments for the X $^1\Sigma^+ \rightarrow$ A $^1\Pi$ system, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 123
Rate constants for vibrational transitions in hydrogen and isotopes, R.E. Kolesnick and G.D. Billing 170 (1993) 201
Calculations of static characteristics of the ionization event in low-energy He(2^3S)–H_2 collisions, J. Vojtík 170 (1993) 209

–small polyatomics
Binding and isomerization energies for the Cu/CN and Cu(I)CN interactions, I. García Cuesta, A. Sánchez de Merás and I. Nebot Gil 170 (1993) 1
Configuration interaction calculations of the vertical electronic spectrum of silane, L. Chantranupong, G. Hirsch, R.J. Buenker and M.A. Dillon 170 (1993) 167

–aromatics
Photophysics of PBD derivatives. I. The fluorescence of para-biphenylyl-substituted 2-(biphenyl-4′-yl)-5-phenyl-1,3,4-oxadiazoles, S. Luňák Jr., M. Nepraš, A. Kurfürst and J. Kuthan 170 (1993) 67
Photophysics of PBD derivatives. II. The character of the lowest excited triplet state of 2-(biphenyl-4′-yl)-5-phenyl-1,3,4-oxadiazole, S. Luňák Jr., M. Nepraš, R. Hrdina, A. Kurfürst and J. Kuthan 170 (1993) 77
Singlet excited-state absorption of eosin Y, A. Penzkofer, A. Beidoun and S. Speiser 170 (1993) 139
Matrix-induced two-photon absorption in anthracene, A. Bree and R. Zwarich 170 (1993) 185
Radiative electron transfer in aryl derivatives of dimethylanilines, J. Herbich and A. Kapturkiewicz 170 (1993) 221

Molecular aggregates
Cavity boundaries in the ab initio polarizable continuum model, F.J. Olivares del Valle, M.A. Aguilar and J.C. Contador 170 (1993) 161

Behavior of the rate constant for reactions in restricted spaces: case of luminescence quenching in water-in-oil microemulsions, P. Lianos, J.C. Brochon and P. Tauc 170 (1993) 235

–van der Waals molecules
Metastable impurity-helium solid phase. Experimental and theoretical evidence, E.B. Gordon, V.V. Khmelenko, A.A. Pelmenev, E.A. Popov, O.F. Pugachev and A.F. Shestakov 170 (1993) 411

–complexes
Binding and isomerization energies for the Cu/CN and Cu(I)CN interactions, I. García Cuesta, A. Sánchez de Merás and I. Nebot Gil 170 (1993) 1

Free radicals (including hydronium and muonium)
Formation of CCl ($A^2\Delta$) by electron impact on $CXCl_3$ (X=H, F, Cl, Br), M. Kusakabe, Y. Ito and I. Tokue 170 (1993) 243
The role of local motions in the kinetic peculiarities of atomic tunneling in solids, V.A. Tolkatchev, V.M. Syutkin and V.L. Vyazovkin 170 (1993) 427

Defects and impurities
Positronium formation and inhibition in binary solid solutions on Al(III) and Co(III) tris(acetylacetonates), J.C. Machado, C.F. Carvalho, W.F. Magalhães, A. Marques Netto, J.Ch. Abbé and G. Duplâtre 170 (1993) 257

Ions and charge carriers
Coordination effects on the stretching vibration of the OH^- ion, K. Hermansson 170 (1993) 177

Phenomena

Molecular structure
Ab initio study of the X $^1\Sigma^+$ and A $^1\Pi$ states of the cyanate anion (NCO^-), Z.-L. Cai 170 (1993) 33
Effects of core correlation on atomic and dimeric phosphorus, L.G.M. Pettersson and B.J. Persson 170 (1993) 149

Vibrations and rotations of molecules
Energy derivative method in MRD CI calculation of rovibrational dependence of nuclear quadrupole coupling constants of diatomic molecules. Application to $^7Li^2H$ in the X $^1\Sigma^+$ and A $^1\Sigma^+$ states, J. Vojtík, I. Paidarová, L. Češpiva and J. Šavrda 170 (1993) 37
Coordination effects on the stretching vibration of the OH^- ion, K. Hermansson 170 (1993) 177

Electronic structure and states
A ligand-field approach for the low-lying states of Ca, Sr and Ba monohalides, A.R. Allouche, G. Wannous and M. Aubert-Frécon 170 (1993) 11
Ab initio study of the X $^1\Sigma^+$ and A $^1\Pi$ states of the cyanate anion (NCO^-), Z.-L. Cai 170 (1993) 33
Photophysics of PBD derivatives. II. The character of the lowest excited triplet state of 2-(biphenyl-4′-yl)-5-phenyl-1,3,4-oxadiazole, S. Luňák Jr., M. Nepraš, R. Hrdina, A. Kurfürst and J. Kuthan 170 (1993) 77

Absolute optical oscillator strengths for discrete and continuum photoabsorption of molecular nitrogen (11–200 eV), W.F. Chan, G. Cooper, R.N.S. Sodhi and C.E. Brion 170 (1993) 81
Absolute optical oscillator strengths for the photoabsorption of molecular oxygen (5–30 eV) at high resolution, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 99
Absolute optical oscillator strengths for the photoabsorption of nitric oxide (5–30 eV) at high resolution, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 111
Absolute optical oscillator strengths for discrete and continuum photoabsorption of carbon monoxide (7–200 eV) and transition moments for the $X\,^1\Sigma^+ \rightarrow A\,^1\Pi$ system, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 123
Configuration interaction calculations of the vertical electronic spectrum of silane, L. Chantranupong, G. Hirsch, R.J. Buenker and M.A. Dillon 170 (1993) 167

Molecular interactions
Cavity boundaries in the ab initio polarizable continuum model, F.J. Olivares del Valle, M.A. Aguilar and J.C. Contador 170 (1993) 161
Coordination effects on the stretching vibration of the OH^- ion, K. Hermansson 170 (1993) 177
Matrix-induced two-photon absorption in anthracene, A. Bree and R. Zwarich 170 (1993) 185
Time correlation functions of liquid OCS. A molecular dynamics simulation study, J. Samios and H. Stassen 170 (1993) 193

Spectral bandshapes and intensities
Absolute optical oscillator strengths for discrete and continuum photoabsorption of molecular nitrogen (11–200 eV), W.F. Chan, G. Cooper, R.N.S. Sodhi and C.E. Brion 170 (1993) 81
Absolute optical oscillator strengths for the photoabsorption of molecular oxygen (5–30 eV) at high resolution, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 99
Absolute optical oscillator strengths for the photoabsorption of nitric oxide (5–30 eV) at high resolution, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 111
Absolute optical oscillator strengths for discrete and continuum photoabsorption of carbon monoxide (7–200 eV) and transition moments for the $X\,^1\Sigma^+ \rightarrow A\,^1\Pi$ system, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 123
Singlet excited-state absorption of eosin Y, A. Penzkofer, A. Beidoun and S. Speiser 170 (1993) 139
Configuration interaction calculations of the vertical electronic spectrum of silane, L. Chantranupong, G. Hirsch, R.J. Buenker and M.A. Dillon 170 (1993) 167

Coupling of electronic and nuclear motion
Intramolecular aspects of the electron transfer in the biferrocenium mixed-valence cation, using PKS theory, K. Boukheddaden, J. Linares, A. Bousseksou, J. Nasser, H. Rabah and F. Varret 170 (1993) 47

Energy transfer processes
The behaviour of trapping after diffusion by tunneling in disordered systems, R. Brown and C. Von Borczyskowski 170 (1993) 57
Rate constants for vibrational transitions in hydrogen and isotopes, R.E. Kolesnick and G.D. Billing 170 (1993) 201

Molecular photophysical processes
Photophysics of PBD derivatives. I. The fluorescence of para-biphenylyl-substituted 2-(biphenyl-4′-yl)-5-phenyl-1,3,4-oxadiazoles, S. Luňák Jr., M. Nepraš, A. Kurfürst and J. Kuthan 170 (1993) 67

Photophysics of PBD derivatives. II. The character of the lowest excited triplet state of 2-(biphenyl-4′-yl)-5-phenyl-1,3,4-oxadiazole, S. Luňák Jr., M. Nepraš, R. Hrdina, A. Kurfürst and J. Kuthan 170 (1993) 77
Absolute optical oscillator strengths for discrete and continuum photoabsorption of molecular nitrogen (11–200 eV), W.F. Chan, G. Cooper, R.N.S. Sodhi and C.E. Brion 170 (1993) 81
Absolute optical oscillator strengths for the photoabsorption of molecular oxygen (5–30 eV) at high resolution, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 99
Absolute optical oscillator strengths for the photoabsorption of nitric oxide (5–30 eV) at high resolution, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 111
Absolute optical oscillator strengths for discrete and continuum photoabsorption of carbon monoxide (7–200 eV) and transition moments for the $X\,^1\Sigma^+ \rightarrow A\,^1\Pi$ system, W.F. Chan, G. Cooper and C.E. Brion 170 (1993) 123
Behavior of the rate constant for reactions in restricted spaces: case of luminescence quenching in water-in-oil microemulsions, P. Lianos, J.C. Brochon and P. Tauc 170 (1993) 235
Intramolecular charge separation and recombination in non-polar environments via long-distance electron transfer through saturated hydrocarbon barriers, J.M. Warman, K.J. Smit, S.A. Jonker, J.W. Verhoeven, H. Oevering, J. Kroon, M.N. Paddon-Row and A.M. Oliver 170 (1993) 359
Tunnel effects on inter- and intramolecular hydrogen transfer reactions of transient dihydro- and hexahydrocarbazoles, U. Kensy, M. Mosquera González and K.H. Grellmann 170 (1993) 381

Intramolecular dynamics
Coordination effects on the stretching vibration of the OH^- ion, K. Hermansson 170 (1993) 177

Luminescence spectra, yields and lifetimes
Photophysics of PBD derivatives. I. The fluorescence of para-biphenylyl-substituted 2-(biphenyl-4′-yl)-5-phenyl-1,3,4-oxadiazoles, S. Luňák Jr., M. Nepraš, A. Kurfürst and J. Kuthan 170 (1993) 67
Photophysics of PBD derivatives. II. The character of the lowest excited triplet state of 2-(biphenyl-4′-yl)-5-phenyl-1,3,4-oxadiazole, S. Luňák Jr., M. Nepraš, R. Hrdina, A. Kurfürst and J. Kuthan 170 (1993) 77

Reactions (including dissociation)
Formation of CCl ($A^2\Delta$) by electron impact on $CXCl_3$ (X=H, F, Cl, Br), M. Kusakabe, Y. Ito and I. Tokue 170 (1993) 243
Dependence of the yield of the short-lived ortho-Ps state on the concentration of CCl_4 in hexane, T. Hirade and O.E. Mogensen 170 (1993) 249
ac-Driven quantum decay, F. Grossmann and P. Hänggi 170 (1993) 295

–gas phase
Binding and isomerization energies for the Cu/CN and Cu(I)CN interactions, I. García Cuesta, A. Sánchez de Merás and I. Nebot Gil 170 (1993) 1
Quantum variational transition state theory revisited, E. Pollak and D. Proselkov 170 (1993) 265

–condensed phase
Dynamical theory of proton tunneling transfer rates in solution: general formulation, D. Borgis and J.T. Hynes 170 (1993) 315

Tunneling dynamics and spatial correlations of long chain growth in solid-state photochlorination of ethylene at low temperatures, C.A. Wight, E.Y. Misochko, E.V. Vetoshkin and V.I. Goldanskii 170 (1993) 393
The role of local motions in the kinetic peculiarities of atomic tunneling in solids, V.A. Tolkatchev, V.M. Syutkin and V.L. Vyazovkin 170 (1993) 427

Tunneling

Electron delocalization and transfer induced by a time-dependent potential: exact treatment of a simple model – transfer, A. Filali-Mouhim, A.-M. Daré, J.-M. Lopez-Castillo and J.-P. Jay-Gerin 170 (1993) 23
The behaviour of trapping after diffusion by tunneling in disordered systems, R. Brown and C. Von Borczyskowski 170 (1993) 57
Quantum variational transition state theory revisited, E. Pollak and D. Proselkov 170 (1993) 265
Quantum chemical dynamics in two dimensions, V.A. Benderskii, D.E. Makarov and P.G. Grinevich 170 (1993) 275
ac-Driven quantum decay, F. Grossmann and P. Hänggi 170 (1993) 295
Asymptotics of many-electron wavefunctions and calculation of tunnel transitions, G.K. Ivanov and M.A. Kozhushner 170 (1993) 303
Dynamical theory of proton tunneling transfer rates in solution: general formulation, D. Borgis and J.T. Hynes 170 (1993) 315
Multimode approach to hydrogen tunneling, Z.K. Smedarchina and W. Siebrand 170 (1993) 347
Intramolecular charge separation and recombination in non-polar environments via long-distance electron transfer through saturated hydrocarbon barriers, J.M. Warman, K.J. Smit, S.A. Jonker, J.W. Verhoeven, H. Oevering, J. Kroon, M.N. Paddon-Row and A.M. Oliver 170 (1993) 359
Tunnel effects on inter- and intramolecular hydrogen transfer reactions of transient dihydro- and hexahydrocarbazoles, U. Kensy, M. Mosquera González and K.H. Grellmann 170 (1993) 381
Tunneling dynamics and spatial correlations of long chain growth in solid-state photochlorination of ethylene at low temperatures, C.A. Wight, E.Y. Misochko, E.V. Vetoshkin and V.I. Goldanskii 170 (1993) 393
Metastable impurity-helium solid phase. Experimental and theoretical evidence, E.B. Gordon, V.V. Khmelenko, A.A. Pelmenev, E.A. Popov, O.F. Pugachev and A.F. Shestakov 170 (1993) 411
The role of local motions in the kinetic peculiarities of atomic tunneling in solids, V.A. Tolkatchev, V.M. Syutkin and V.L. Vyazovkin 170 (1993) 427
Thermally activated configurational tunneling at trapping and recombination in glassy semiconductors, M.I. Klinger and S.N. Taraskin 170 (1993) 437

Electron transfer

Electron delocalization and transfer induced by a time-dependent potential: exact treatment of a simple model – transfer, A. Filali-Mouhim, A.-M. Daré, J.-M. Lopez-Castillo and J.-P. Jay-Gerin 170 (1993) 23
Intramolecular aspects of the electron transfer in the biferrocenium mixed-valence cation, using PKS theory, K. Boukheddaden, J. Linares, A. Bousseksou, J. Nasser, H. Rabah and F. Varret 170 (1993) 47
Radiative electron transfer in aryl derivatives of dimethylanilines, J. Herbich and A. Kapturkiewicz 170 (1993) 221

Intramolecular charge separation and recombination in non-polar environments via long-distance electron transfer through saturated hydrocarbon barriers, J.M. Warman, K.J. Smit, S.A. Jonker, J.W. Verhoeven, H. Oevering, J. Kroon, M.N. Paddon-Row and A.M. Oliver 170 (1993) 359

Positron annihilation

Dependence of the yield of the short-lived ortho-Ps state on the concentration of CCl_4 in hexane, T. Hirade and O.E. Mogensen 170 (1993) 249

Positronium formation and inhibition in binary solid solutions on Al(III) and Co(III) tris(acetylacetonates), J.C. Machado, C.F. Carvalho, W.F. Magalhães, A. Marques Netto, J.Ch. Abbé and G. Duplâtre 170 (1993) 257

Ionization (including Rydberg states)

Configuration interaction calculations of the vertical electronic spectrum of silane, L. Chantranupong, G. Hirsch, R.J. Buenker and M.A. Dillon 170 (1993) 167

Calculations of static characteristics of the ionization event in low-energy $He(2^3S)$–H_2 collisions, J. Vojtík 170 (1993) 209

Molecular motion (including diffusive)

Time correlation functions of liquid OCS. A molecular dynamics simulation study, J. Samios and H. Stassen 170 (1993) 193

Behavior of the rate constant for reactions in restricted spaces: case of luminescence quenching in water-in-oil microemulsions, P. Lianos, J.C. Brochon and P. Tauc 170 (1993) 235

Quantum variational transition state theory revisited, E. Pollak and D. Proselkov 170 (1993) 265

Isotopic effects

Tunnel effects on inter- and intramolecular hydrogen transfer reactions of transient dihydro- and hexahydrocarbazoles, U. Kensy, M. Mosquera González and K.H. Grellmann 170 (1993) 381

Structure of solids and liquids

Metastable impurity-helium solid phase. Experimental and theoretical evidence, E.B. Gordon, V.V. Khmelenko, A.A. Pelmenev, E.A. Popov, O.F. Pugachev and A.F. Shestakov 170 (1993) 411